Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:17 PM GMT

PDB ID	:	1O9L
Title	:	SUCCINATE:COENZYME-A TRANSFERASE (PIG HEART)
Authors	:	Mitchell, E.P.; Lloyd, A.J.; Lewis, G.; Shoolingin-Jordan, P.
Deposited on	:	2002-12-17
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

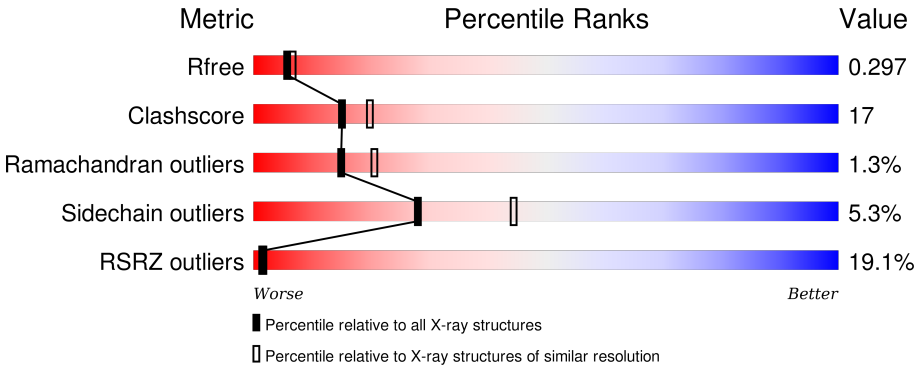
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	481	20% 66% 28%
1	B	481	17% 65% 21% 12%
1	C	481	16% 60% 25% 12%
1	D	481	17% 66% 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EMC	A	9003	-	-	-	X
2	EMC	D	9000	-	-	-	X
2	EMC	D	9001	-	-	-	X
2	EMC	D	9002	-	-	-	X
3	EMT	A	9007	-	-	X	X
3	EMT	B	9008	-	-	X	X

2 Entry composition

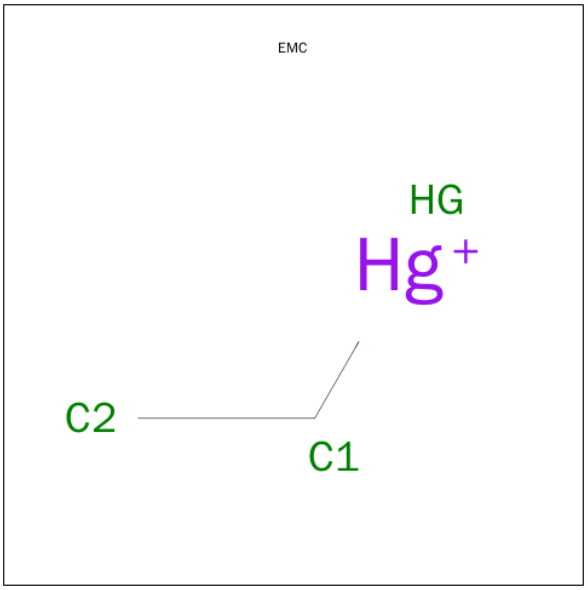
There are 4 unique types of molecules in this entry. The entry contains 14135 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SUCCINYL-COA\:3-KETOACID-COENZYME A TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3568	2264	612	674	18			
1	B	425	Total	C	N	O	S	0	0	0
			3239	2056	554	616	13			
1	C	425	Total	C	N	O	S	0	0	0
			3234	2053	553	614	14			
1	D	464	Total	C	N	O	S	0	0	0
			3535	2244	604	669	18			

- Molecule 2 is ETHYL MERCURY ION (three-letter code: EMC) (formula: C_2H_5Hg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	Hg	0	0
			3	2	1		
2	B	1	Total	C	Hg	0	0
			3	2	1		

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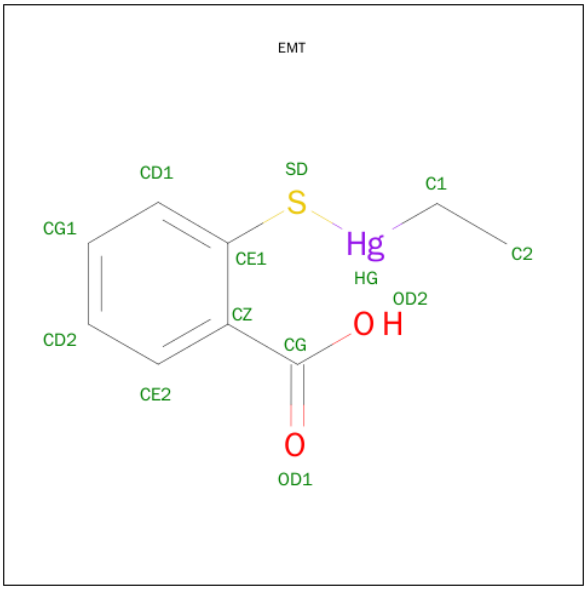
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C Hg 3 2 1	0	0
2	C	1	Total C Hg 3 2 1	0	0
2	D	1	Total C Hg 3 2 1	0	0
2	D	1	Total C Hg 3 2 1	0	0
2	D	1	Total C Hg 3 2 1	0	0

- Molecule 3 is 2-(ETHYLMERCURI-THIO)-BENZOIC ACID (three-letter code: EMT) (formula: $C_9H_{10}HgO_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Hg O S 13 9 1 2 1	0	0
3	B	1	Total C Hg O S 13 9 1 2 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	107	Total O 107 107	0	0
4	B	86	Total O 86 86	0	0

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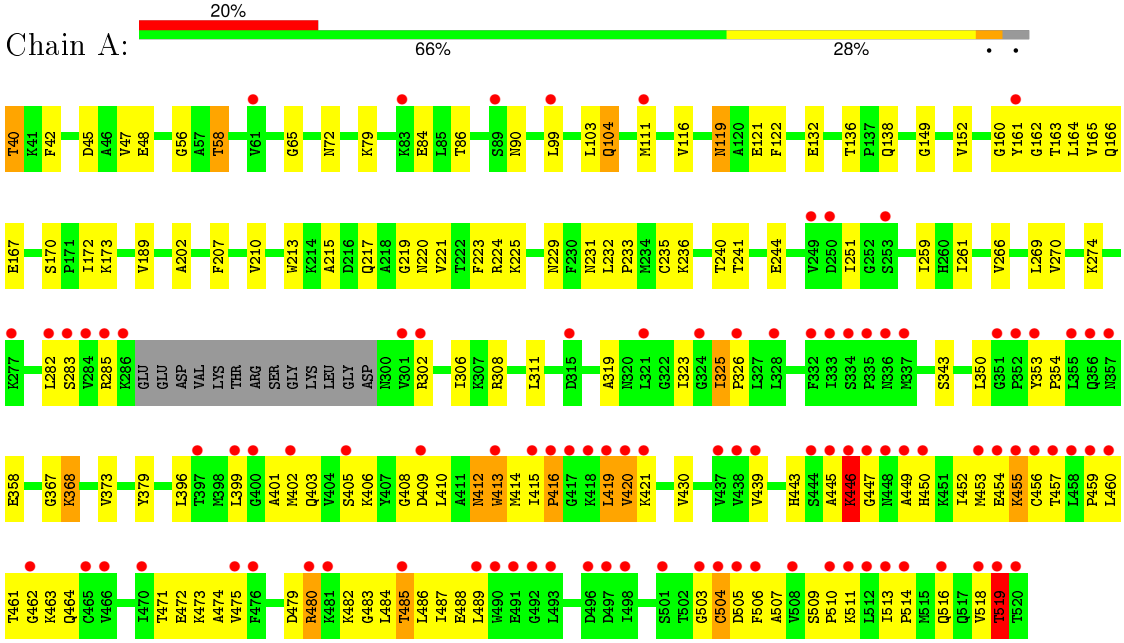
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	139	Total O 139 139	0	0
4	D	180	Total O 180 180	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

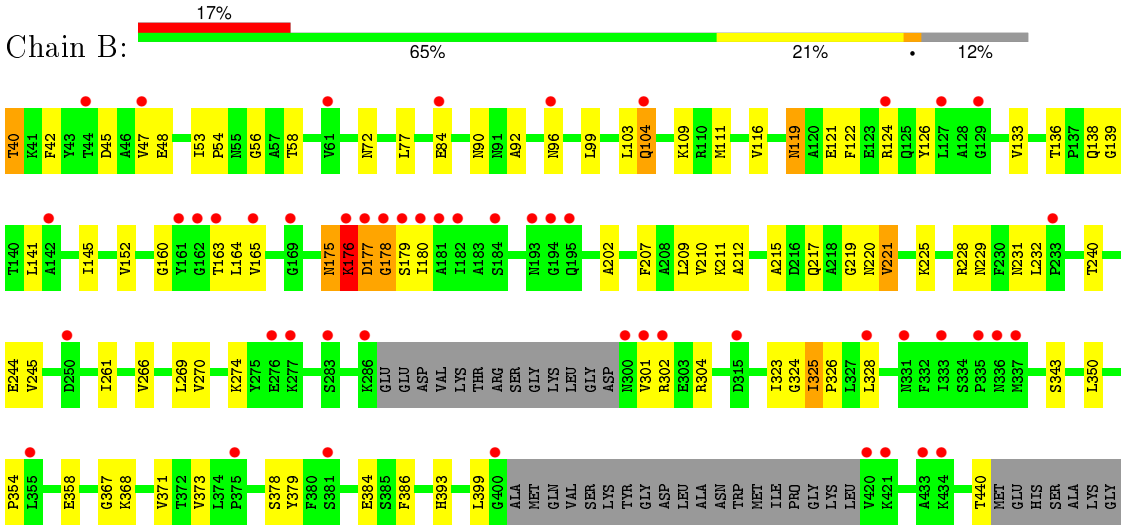
- Molecule 1: SUCCINYL-COA\:3-KETOACID-COENZYME A TRANSFERASE

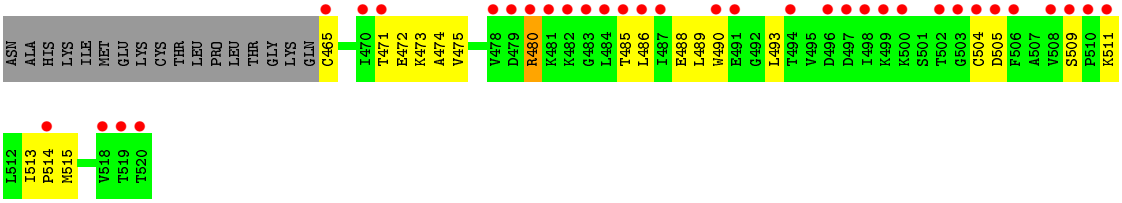
Chain A:



- Molecule 1: SUCCINYL-COA\:3-KETOACID-COENZYME A TRANSFERASE

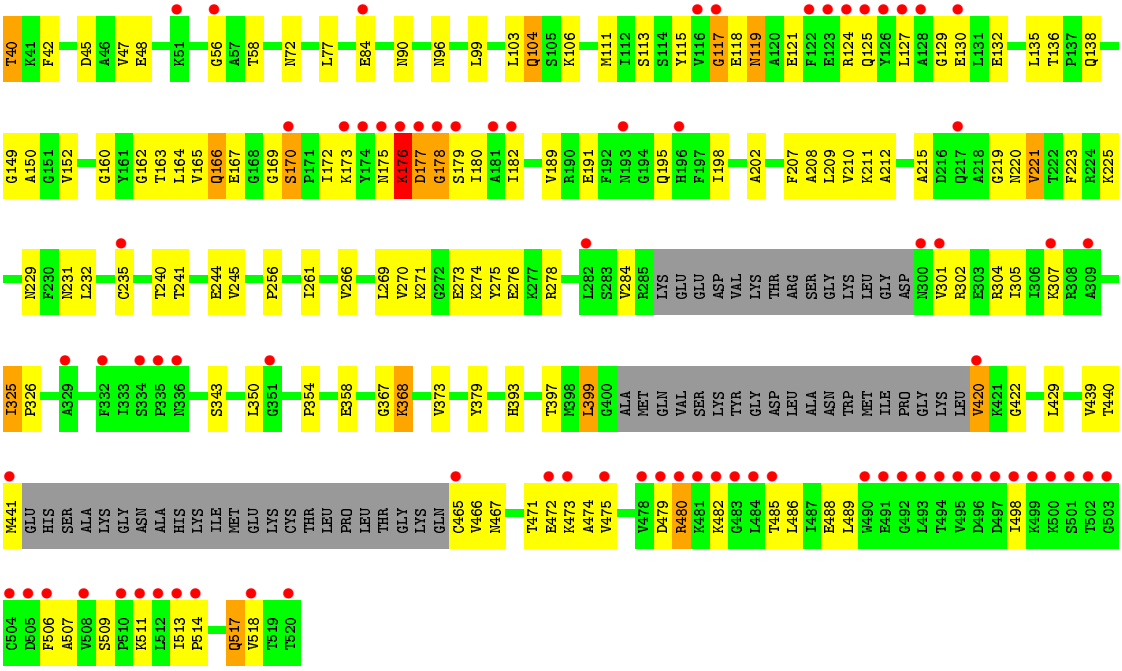
Chain B:

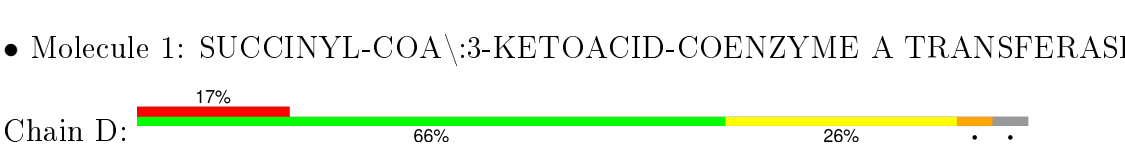


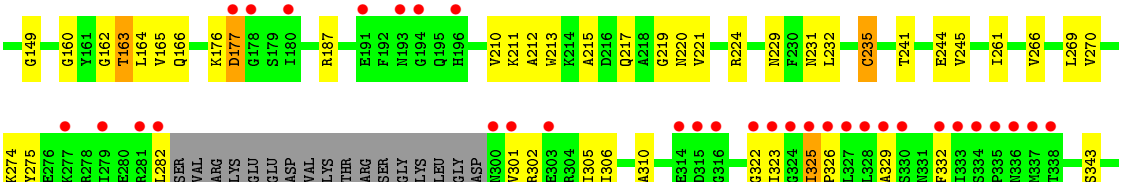


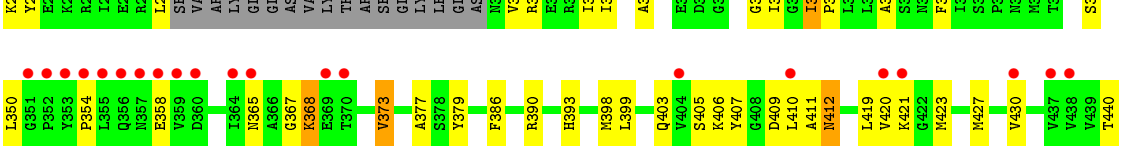
• Molecule 1: SUCCINYL-COA\:3-KETOACID-COENZYME A TRANSFERASE

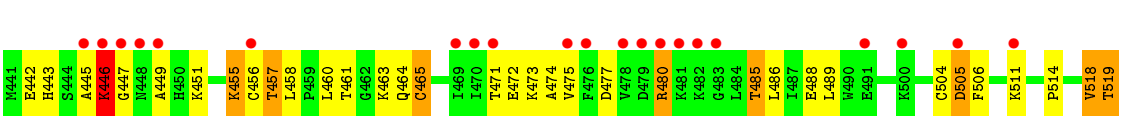
Chain C:











• Molecule 1: SUCCINYL-COA\:3-KETOACID-COENZYME A TRANSFERASE

Chain D:


T520

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.80Å 133.80Å 101.90Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	29.76 – 2.40 29.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.76-2.40) 99.8 (29.76-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.06 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.270 0.277 , 0.297	Depositor DCC
R_{free} test set	1506 reflections (2.03%)	DCC
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 69.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 75610 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14135	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EMT, EMC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/3626	0.63	0/4894
1	B	0.36	0/3288	0.61	0/4438
1	C	0.40	0/3283	0.64	1/4431 (0.0%)
1	D	0.42	0/3593	0.66	1/4851 (0.0%)
All	All	0.39	0/13790	0.64	2/18614 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	465	CYS	CA-CB-SG	6.20	125.17	114.00
1	D	505	ASP	N-CA-C	-5.21	96.93	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3568	0	3639	137	0
1	B	3239	0	3296	87	0
1	C	3234	0	3281	119	0
1	D	3535	0	3597	133	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	0	0
2	C	6	0	0	0	0
2	D	9	0	0	1	0
3	A	13	0	4	9	0
3	B	13	0	4	8	0
4	A	107	0	0	6	0
4	B	86	0	0	6	0
4	C	139	0	0	10	0
4	D	180	0	0	5	0
All	All	14135	0	13821	480	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (480) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9008:EMT:HE2	3:B:9008:EMT:CZ	2.07	1.23
3:B:9008:EMT:HE2	3:B:9008:EMT:CD2	2.06	1.23
3:A:9007:EMT:HE2	3:A:9007:EMT:CD2	2.06	1.21
3:A:9007:EMT:HE2	3:A:9007:EMT:CZ	2.06	1.21
1:B:163:THR:HG22	1:B:165:VAL:H	1.13	1.10
1:A:163:THR:HG22	1:A:165:VAL:H	1.17	1.10
3:A:9007:EMT:HE2	3:A:9007:EMT:CE2	0.97	1.06
1:C:163:THR:HG22	1:C:165:VAL:H	1.12	1.06
3:B:9008:EMT:HE2	3:B:9008:EMT:CE2	0.97	1.06
1:C:96:ASN:HB3	4:C:2018:HOH:O	1.59	1.02
1:D:163:THR:HG22	1:D:165:VAL:H	1.25	1.01
1:D:325:ILE:HD13	1:D:440:THR:HB	1.41	1.00
1:B:96:ASN:HB3	4:B:2011:HOH:O	1.60	0.99
1:D:446:LYS:HG2	1:D:447:GLY:H	1.26	0.99
1:C:307:LYS:HE3	1:C:517:GLN:HG3	1.50	0.94
1:B:40:THR:HG21	1:B:219:GLY:HA3	1.53	0.90
1:A:445:ALA:HB3	1:A:449:ALA:HB3	1.54	0.90
1:A:325:ILE:HG23	1:A:326:PRO:HD3	1.54	0.88
1:A:450:HIS:ND1	1:A:503:GLY:HA2	1.88	0.88
1:D:306:ILE:HA	1:D:325:ILE:HG13	1.57	0.87
1:D:40:THR:HB	1:D:266:VAL:O	1.75	0.86
1:B:325:ILE:HG23	1:B:326:PRO:HD3	1.57	0.85
1:D:403:GLN:HE22	1:D:457:THR:H	1.23	0.85
1:D:40:THR:HG21	1:D:219:GLY:HA3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:THR:HB	1:C:266:VAL:O	1.76	0.84
1:A:162:GLY:H	1:A:166:GLN:NE2	1.76	0.84
1:A:40:THR:HG21	1:A:219:GLY:HA3	1.59	0.84
1:A:406:LYS:HE3	1:C:273:GLU:HG2	1.60	0.83
1:B:40:THR:HB	1:B:266:VAL:O	1.78	0.83
1:C:325:ILE:HG23	1:C:326:PRO:HD3	1.61	0.82
1:D:116:VAL:HG11	1:D:122:PHE:CZ	2.15	0.82
1:D:471:THR:CG2	1:D:474:ALA:H	1.92	0.81
1:D:445:ALA:HB3	1:D:449:ALA:HB3	1.61	0.81
1:B:221:VAL:HG22	1:B:261:ILE:HB	1.62	0.80
1:A:40:THR:HB	1:A:266:VAL:O	1.81	0.80
1:A:410:LEU:HG	1:A:461:THR:HB	1.63	0.80
1:C:221:VAL:HG22	1:C:261:ILE:HB	1.64	0.79
1:C:40:THR:HG21	1:C:219:GLY:HA3	1.62	0.79
1:C:325:ILE:HG22	4:C:2091:HOH:O	1.82	0.78
1:D:221:VAL:HG22	1:D:261:ILE:HB	1.64	0.77
1:A:221:VAL:HG22	1:A:261:ILE:HB	1.67	0.76
1:D:305:ILE:HB	1:D:325:ILE:HD12	1.67	0.76
1:A:446:LYS:HG2	1:A:447:GLY:H	1.49	0.76
1:C:162:GLY:H	1:C:166:GLN:NE2	1.85	0.75
1:A:471:THR:HG23	1:A:474:ALA:H	1.53	0.73
1:A:443:HIS:ND1	1:A:471:THR:HG21	2.02	0.73
1:A:401:ALA:HA	1:A:412:ASN:HB3	1.71	0.72
1:C:56:GLY:HA2	1:C:84:GLU:O	1.89	0.72
1:B:325:ILE:HD13	1:B:440:THR:HB	1.72	0.72
1:D:305:ILE:HG22	1:D:325:ILE:CD1	2.19	0.71
1:D:464:GLN:NE2	1:D:480:ARG:HB2	2.06	0.71
1:C:164:LEU:O	1:C:167:GLU:O	2.09	0.71
1:C:132:GLU:HG2	1:C:173:LYS:HB2	1.73	0.70
1:A:511:LYS:N	1:A:511:LYS:HD2	2.07	0.70
1:A:162:GLY:H	1:A:166:GLN:HE21	1.38	0.69
1:A:456:CYS:SG	1:A:460:LEU:HG	2.33	0.69
1:D:475:VAL:HB	1:D:488:GLU:HB2	1.73	0.69
1:C:511:LYS:HD2	1:C:511:LYS:N	2.09	0.68
1:D:305:ILE:CB	1:D:325:ILE:HD12	2.23	0.68
1:A:475:VAL:HB	1:A:488:GLU:HB2	1.74	0.68
1:B:475:VAL:HB	1:B:488:GLU:HB2	1.74	0.68
1:C:96:ASN:ND2	4:C:2019:HOH:O	2.27	0.68
1:A:42:PHE:CE2	1:A:269:LEU:HD23	2.29	0.68
1:A:56:GLY:HA2	1:A:84:GLU:O	1.94	0.68
3:B:9008:EMT:HD1	4:B:2075:HOH:O	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:GLN:NE2	1:D:457:THR:H	1.93	0.67
1:A:445:ALA:HB1	1:A:446:LYS:HD3	1.77	0.66
1:D:325:ILE:HG23	1:D:326:PRO:HD3	1.76	0.66
1:B:163:THR:HG22	1:B:165:VAL:N	1.98	0.66
1:B:472:GLU:HG3	1:B:473:LYS:HG3	1.77	0.66
1:D:455:LYS:H	1:D:455:LYS:HD3	1.60	0.66
1:B:42:PHE:CE2	1:B:269:LEU:HD23	2.30	0.66
1:C:475:VAL:HB	1:C:488:GLU:HB2	1.78	0.66
1:C:479:ASP:HB3	1:C:482:LYS:HB2	1.78	0.65
1:D:446:LYS:HG2	1:D:447:GLY:N	2.05	0.65
1:A:172:ILE:HG12	3:A:9007:EMT:HD1	1.77	0.65
1:B:489:LEU:O	1:B:514:PRO:HA	1.95	0.65
1:A:414:MET:CE	1:A:459:PRO:HG2	2.27	0.65
1:D:471:THR:HG22	1:D:474:ALA:H	1.62	0.65
1:A:471:THR:CG2	1:A:474:ALA:H	2.10	0.64
1:A:511:LYS:O	1:A:513:ILE:HG23	1.97	0.64
1:A:403:GLN:HE22	1:A:457:THR:N	1.95	0.64
1:A:450:HIS:CG	1:A:503:GLY:HA2	2.31	0.64
1:D:117:GLY:O	1:D:118:GLU:HB2	1.95	0.64
1:C:471:THR:HG22	1:C:474:ALA:O	1.97	0.64
1:A:160:GLY:O	1:A:163:THR:HB	1.98	0.64
1:A:455:LYS:HE2	1:A:455:LYS:O	1.98	0.64
1:B:511:LYS:N	1:B:511:LYS:HD2	2.12	0.64
1:C:354:PRO:HB2	1:C:358:GLU:HB2	1.79	0.64
1:C:211:LYS:HE2	1:C:275:TYR:CE1	2.33	0.64
1:D:410:LEU:HD12	1:D:411:ALA:N	2.13	0.63
1:D:116:VAL:HG22	1:D:421:LYS:O	1.99	0.63
1:A:119:ASN:HD22	1:A:119:ASN:C	2.02	0.63
1:A:472:GLU:HG3	1:A:473:LYS:HG3	1.80	0.63
3:A:9007:EMT:HE2	3:A:9007:EMT:CG	2.67	0.63
1:D:45:ASP:OD2	1:D:48:GLU:HG2	1.99	0.63
3:B:9008:EMT:HE2	3:B:9008:EMT:CG	2.67	0.62
1:C:471:THR:HG23	1:C:474:ALA:H	1.64	0.62
1:D:403:GLN:HE22	1:D:457:THR:N	1.97	0.62
1:D:511:LYS:HD2	1:D:511:LYS:N	2.14	0.62
1:A:104:GLN:NE2	1:A:121:GLU:HG2	2.15	0.62
1:B:116:VAL:HG21	1:B:122:PHE:CE2	2.35	0.62
1:C:472:GLU:HG3	1:C:473:LYS:HG3	1.80	0.62
1:A:79:LYS:HE3	4:A:2010:HOH:O	1.98	0.62
1:C:163:THR:HG22	1:C:165:VAL:N	1.98	0.62
1:D:163:THR:HG22	1:D:165:VAL:N	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:LYS:HE3	1:D:407:TYR:CE2	2.35	0.61
1:D:471:THR:HG23	1:D:474:ALA:H	1.65	0.61
1:D:119:ASN:HD22	1:D:119:ASN:C	2.02	0.61
1:C:511:LYS:O	1:C:513:ILE:HG23	2.01	0.61
1:D:406:LYS:HE3	1:D:407:TYR:CZ	2.35	0.61
1:C:441:MET:HE1	4:C:2135:HOH:O	2.00	0.61
1:C:45:ASP:OD2	1:C:48:GLU:HG2	2.00	0.60
1:A:446:LYS:N	1:A:446:LYS:HD3	2.15	0.60
1:A:104:GLN:HG2	4:A:2015:HOH:O	2.01	0.60
1:C:42:PHE:CE2	1:C:269:LEU:HD23	2.35	0.60
1:B:302:ARG:HG2	4:B:2050:HOH:O	2.01	0.60
1:D:126:TYR:CE1	1:D:133:VAL:HG13	2.37	0.60
1:D:301:VAL:HG13	1:D:472:GLU:HB3	1.84	0.60
1:B:471:THR:HG22	1:B:474:ALA:O	2.02	0.60
1:A:163:THR:HG22	1:A:165:VAL:N	2.02	0.60
1:C:115:TYR:CZ	1:C:117:GLY:HA3	2.37	0.60
1:B:56:GLY:HA2	1:B:84:GLU:O	2.01	0.59
1:B:160:GLY:O	1:B:163:THR:HB	2.02	0.59
1:A:401:ALA:HA	1:A:412:ASN:CB	2.33	0.59
1:C:45:ASP:OD1	1:C:47:VAL:HG12	2.02	0.59
1:D:354:PRO:HB2	1:D:358:GLU:HB2	1.85	0.59
1:C:471:THR:CG2	1:C:474:ALA:H	2.16	0.59
1:C:106:LYS:HG2	1:C:125:GLN:HE22	1.67	0.59
1:A:452:ILE:HG22	1:A:484:LEU:HD11	1.85	0.59
1:C:90:ASN:ND2	1:C:138:GLN:HG3	2.18	0.59
1:B:119:ASN:HD22	1:B:119:ASN:C	2.05	0.59
1:C:307:LYS:HE3	1:C:517:GLN:CG	2.29	0.59
1:D:116:VAL:HG21	1:D:122:PHE:CE1	2.37	0.58
1:D:446:LYS:CG	1:D:447:GLY:H	2.05	0.58
1:A:454:GLU:HB2	1:A:504:CYS:SG	2.43	0.58
1:A:413:TRP:CE3	1:A:414:MET:HB2	2.38	0.58
1:A:474:ALA:HB1	1:A:486:LEU:CD1	2.33	0.58
1:B:471:THR:CG2	1:B:474:ALA:H	2.17	0.58
1:D:211:LYS:HE2	1:D:275:TYR:CE1	2.39	0.58
1:D:443:HIS:ND1	1:D:471:THR:HG21	2.19	0.58
1:C:160:GLY:O	1:C:163:THR:HB	2.04	0.57
1:B:211:LYS:HE3	4:B:2006:HOH:O	2.05	0.57
1:D:480:ARG:H	1:D:480:ARG:CZ	2.18	0.57
1:A:489:LEU:O	1:A:514:PRO:HA	2.03	0.57
1:A:132:GLU:CG	1:A:173:LYS:HD2	2.35	0.57
1:C:474:ALA:HB1	1:C:486:LEU:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:TYR:CD1	1:D:133:VAL:CG1	2.88	0.57
1:D:310:ALA:HA	1:D:329:ALA:HB1	1.86	0.57
1:B:354:PRO:HB2	1:B:358:GLU:HB2	1.85	0.57
1:C:90:ASN:HD21	1:C:138:GLN:HG3	1.70	0.56
1:C:325:ILE:HD13	1:C:440:THR:HB	1.87	0.56
1:B:104:GLN:NE2	1:B:121:GLU:HG2	2.20	0.56
1:A:45:ASP:OD1	1:A:47:VAL:HG12	2.05	0.56
1:D:99:LEU:HD23	1:D:111:MET:CE	2.35	0.56
1:D:124:ARG:HH12	1:D:125:GLN:HG2	1.70	0.56
1:A:45:ASP:OD2	1:A:48:GLU:HG2	2.06	0.56
1:C:118:GLU:O	1:C:119:ASN:HB2	2.05	0.56
1:D:472:GLU:HG3	1:D:473:LYS:HG3	1.87	0.56
1:B:471:THR:HG23	1:B:474:ALA:H	1.70	0.56
1:C:367:GLY:O	1:C:368:LYS:HB2	2.06	0.55
1:C:106:LYS:HG2	1:C:125:GLN:NE2	2.21	0.55
1:C:99:LEU:HD23	1:C:111:MET:CE	2.36	0.55
3:A:9007:EMT:SD	3:A:9007:EMT:OD1	2.65	0.55
1:D:471:THR:HG23	1:D:473:LYS:H	1.71	0.55
1:A:99:LEU:HD23	1:A:111:MET:CE	2.37	0.55
1:A:446:LYS:H	1:A:446:LYS:HD3	1.72	0.55
1:A:455:LYS:HZ3	1:A:455:LYS:H	1.54	0.55
1:D:305:ILE:CG2	1:D:325:ILE:HD12	2.37	0.54
1:A:509:SER:C	1:A:511:LYS:H	2.10	0.54
1:A:455:LYS:H	1:A:455:LYS:NZ	2.04	0.54
1:D:471:THR:HG22	1:D:474:ALA:O	2.08	0.54
1:D:310:ALA:CA	1:D:329:ALA:HB1	2.37	0.54
1:A:408:GLY:HA3	1:A:464:GLN:HA	1.89	0.54
1:A:232:LEU:HG	1:A:261:ILE:HD11	1.89	0.54
1:C:343:SER:HB2	1:C:350:LEU:HD11	1.89	0.54
1:B:490:TRP:HB3	1:B:493:LEU:HD12	1.89	0.54
1:C:397:THR:HG21	1:C:429:LEU:HB3	1.89	0.54
1:C:489:LEU:O	1:C:514:PRO:HA	2.08	0.54
1:A:164:LEU:HA	1:A:167:GLU:HB2	1.89	0.54
1:A:413:TRP:HD1	1:A:461:THR:HG1	1.54	0.54
1:B:325:ILE:CD1	1:B:440:THR:HB	2.36	0.53
1:D:90:ASN:ND2	1:D:138:GLN:HG3	2.23	0.53
1:D:305:ILE:CG2	1:D:325:ILE:CD1	2.87	0.53
1:D:90:ASN:HD21	1:D:138:GLN:HG3	1.74	0.53
1:D:211:LYS:HE3	4:D:2015:HOH:O	2.08	0.53
1:D:343:SER:HB2	1:D:350:LEU:HD11	1.91	0.53
1:A:72:ASN:HD21	1:A:274:LYS:H	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LYS:N	1:C:176:LYS:HD3	2.23	0.53
1:D:412:ASN:C	1:D:412:ASN:HD22	2.11	0.53
1:A:456:CYS:SG	1:A:456:CYS:O	2.66	0.53
1:D:405:SER:OG	1:D:409:ASP:HB2	2.09	0.53
1:A:406:LYS:NZ	1:A:454:GLU:HG3	2.24	0.53
1:A:414:MET:HE2	1:A:459:PRO:HG2	1.88	0.53
1:D:446:LYS:NZ	1:D:449:ALA:HB2	2.24	0.53
1:A:90:ASN:HD21	1:A:138:GLN:HG3	1.73	0.53
1:D:489:LEU:O	1:D:514:PRO:HA	2.09	0.52
1:D:42:PHE:CE2	1:D:269:LEU:HD23	2.44	0.52
1:B:474:ALA:HB1	1:B:486:LEU:CD1	2.40	0.52
1:A:474:ALA:HB1	1:A:486:LEU:HD11	1.91	0.52
1:C:176:LYS:HG2	1:C:177:ASP:N	2.24	0.52
1:D:72:ASN:HD21	1:D:274:LYS:H	1.56	0.52
1:B:99:LEU:HD23	1:B:111:MET:HE1	1.91	0.52
3:A:9007:EMT:OD2	3:A:9007:EMT:HE2	2.48	0.52
1:B:511:LYS:O	1:B:513:ILE:HG23	2.08	0.52
1:D:306:ILE:HG12	1:D:325:ILE:HA	1.92	0.52
1:D:367:GLY:O	1:D:368:LYS:HB2	2.09	0.52
1:C:180:ILE:HD12	1:C:180:ILE:N	2.23	0.52
1:B:176:LYS:N	1:B:176:LYS:HD3	2.25	0.52
1:D:471:THR:HG23	1:D:473:LYS:N	2.25	0.52
1:A:479:ASP:OD2	1:A:482:LYS:HG3	2.09	0.52
1:C:480:ARG:HH11	1:C:480:ARG:HG3	1.74	0.52
1:D:455:LYS:HD3	1:D:455:LYS:N	2.25	0.51
1:C:301:VAL:HG13	1:C:472:GLU:HB3	1.93	0.51
1:A:354:PRO:HB2	1:A:358:GLU:HB2	1.92	0.51
3:B:9008:EMT:HE2	3:B:9008:EMT:OD2	2.48	0.51
1:D:326:PRO:HA	1:D:398:MET:CE	2.40	0.51
1:C:135:LEU:HD13	1:C:422:GLY:HA2	1.91	0.51
1:C:99:LEU:HD23	1:C:111:MET:HE1	1.91	0.51
1:A:414:MET:HE1	1:A:459:PRO:HG2	1.92	0.51
1:C:393:HIS:HE1	1:D:149:GLY:O	1.93	0.51
1:B:72:ASN:HD21	1:B:274:LYS:H	1.59	0.51
1:A:166:GLN:OE1	1:A:189:VAL:HG21	2.11	0.51
1:C:169:GLY:O	1:C:170:SER:C	2.49	0.51
1:D:235:CYS:O	1:D:241:THR:HG21	2.11	0.51
1:C:302:ARG:HG2	4:C:2084:HOH:O	2.10	0.51
1:A:406:LYS:HZ1	1:A:454:GLU:HG3	1.76	0.51
1:B:119:ASN:HD21	1:B:121:GLU:HB3	1.76	0.51
1:A:132:GLU:HG2	1:A:173:LYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:THR:CG2	1:A:164:LEU:N	2.73	0.51
1:C:163:THR:CG2	1:C:164:LEU:N	2.74	0.50
1:D:160:GLY:O	1:D:163:THR:HB	2.11	0.50
1:B:232:LEU:HG	1:B:261:ILE:HD11	1.92	0.50
1:B:45:ASP:OD2	1:B:48:GLU:HG2	2.11	0.50
1:B:504:CYS:SG	1:B:505:ASP:N	2.84	0.50
1:A:472:GLU:HG3	1:A:473:LYS:N	2.27	0.50
1:B:163:THR:CG2	1:B:164:LEU:N	2.75	0.50
1:A:446:LYS:HG2	1:A:447:GLY:N	2.24	0.50
1:C:474:ALA:HB1	1:C:486:LEU:HD11	1.94	0.50
1:D:163:THR:HG21	1:D:427:MET:CE	2.41	0.50
1:B:302:ARG:NH1	4:B:2049:HOH:O	2.43	0.50
1:A:65:GLY:HA3	1:A:368:LYS:HD2	1.94	0.50
1:A:518:VAL:O	1:A:519:THR:HG23	2.12	0.50
1:C:149:GLY:O	1:D:393:HIS:HE1	1.94	0.49
1:D:430:VAL:HB	1:D:465:CYS:HB3	1.94	0.49
1:A:410:LEU:HD11	1:A:430:VAL:HG11	1.94	0.49
1:A:402:MET:HE2	1:A:412:ASN:HA	1.93	0.49
1:D:124:ARG:NH2	1:D:130:GLU:OE2	2.43	0.49
1:B:45:ASP:OD1	1:B:47:VAL:HG12	2.13	0.49
1:A:415:ILE:HB	1:A:419:LEU:HB2	1.95	0.49
1:C:276:GLU:O	1:C:278:ARG:N	2.44	0.49
1:D:176:LYS:O	1:D:177:ASP:HB3	2.11	0.49
1:A:406:LYS:HA	1:A:484:LEU:HG	1.94	0.49
1:A:149:GLY:O	1:B:393:HIS:HE1	1.96	0.49
1:D:176:LYS:O	1:D:177:ASP:CB	2.61	0.49
1:B:244:GLU:HA	1:B:270:VAL:O	2.12	0.49
1:B:180:ILE:HD12	1:B:180:ILE:N	2.27	0.49
1:C:479:ASP:OD2	1:C:482:LYS:HG3	2.12	0.49
1:D:45:ASP:OD2	1:D:47:VAL:HG13	2.12	0.49
1:C:121:GLU:O	1:C:125:GLN:HG3	2.13	0.49
1:C:420:VAL:HB	4:C:2121:HOH:O	2.13	0.49
1:C:368:LYS:HG3	4:C:2010:HOH:O	2.13	0.49
1:A:302:ARG:O	1:A:306:ILE:HG13	2.12	0.49
1:A:325:ILE:CG2	1:A:326:PRO:HD3	2.35	0.49
1:C:175:ASN:HB2	1:C:179:SER:OG	2.12	0.49
1:C:480:ARG:NH1	1:C:480:ARG:HG3	2.28	0.49
1:D:213:TRP:CE2	1:D:224:ARG:HD2	2.47	0.49
1:A:319:ALA:HA	1:A:396:LEU:O	2.12	0.48
1:C:176:LYS:HZ2	1:C:178:GLY:N	2.12	0.48
1:D:65:GLY:HA2	4:D:2123:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:CYS:SG	1:D:505:ASP:N	2.86	0.48
1:C:215:ALA:HA	1:C:220:ASN:O	2.13	0.48
1:D:325:ILE:HD13	1:D:440:THR:CB	2.29	0.48
1:A:480:ARG:H	1:A:480:ARG:CZ	2.26	0.48
1:B:509:SER:C	1:B:511:LYS:H	2.16	0.48
1:A:90:ASN:ND2	1:A:138:GLN:HG3	2.28	0.48
1:A:343:SER:HB2	1:A:350:LEU:HD11	1.95	0.48
1:D:163:THR:CG2	1:D:164:LEU:N	2.76	0.48
1:A:471:THR:HG22	1:A:474:ALA:O	2.14	0.48
1:A:215:ALA:HA	1:A:220:ASN:O	2.13	0.48
1:D:323:ILE:HG21	1:D:367:GLY:HA3	1.95	0.48
1:B:175:ASN:O	1:B:177:ASP:N	2.47	0.48
1:C:393:HIS:HD2	4:D:2121:HOH:O	1.97	0.48
1:A:213:TRP:CE2	1:A:224:ARG:HD2	2.48	0.48
1:D:104:GLN:CA	1:D:104:GLN:HE21	2.27	0.48
1:A:450:HIS:HB3	1:A:503:GLY:CA	2.44	0.48
1:B:480:ARG:H	1:B:480:ARG:CZ	2.26	0.48
1:C:304:ARG:HA	1:C:517:GLN:OE1	2.14	0.47
1:C:176:LYS:HE3	1:C:179:SER:OG	2.13	0.47
1:D:412:ASN:C	1:D:412:ASN:ND2	2.66	0.47
1:D:56:GLY:HA2	1:D:84:GLU:O	2.13	0.47
1:C:325:ILE:CG2	1:C:326:PRO:HD3	2.41	0.47
1:C:284:VAL:HG13	1:C:354:PRO:O	2.14	0.47
1:D:456:CYS:SG	1:D:460:LEU:HD21	2.55	0.47
1:D:162:GLY:HA3	1:D:463:LYS:HD3	1.97	0.47
1:A:170:SER:HB3	3:A:9007:EMT:SD	2.54	0.47
1:A:161:TYR:CE2	1:A:463:LYS:HE2	2.50	0.47
1:A:410:LEU:O	1:A:461:THR:N	2.41	0.47
1:B:177:ASP:CG	1:B:178:GLY:H	2.18	0.47
1:C:176:LYS:O	1:C:177:ASP:HB2	2.14	0.47
1:C:72:ASN:HD21	1:C:274:LYS:H	1.63	0.47
1:D:480:ARG:HH11	1:D:480:ARG:HB3	1.80	0.47
1:A:403:GLN:HE22	1:A:457:THR:H	1.59	0.47
1:B:215:ALA:CB	1:B:269:LEU:HD21	2.44	0.47
1:D:215:ALA:HA	1:D:220:ASN:O	2.15	0.47
1:C:166:GLN:OE1	1:C:189:VAL:HG21	2.15	0.46
1:B:465:CYS:SG	3:B:9008:EMT:CE2	3.03	0.46
1:A:302:ARG:HG2	4:A:2067:HOH:O	2.13	0.46
1:A:406:LYS:O	1:A:483:GLY:HA2	2.15	0.46
1:C:212:ALA:HB3	1:C:245:VAL:HG12	1.97	0.46
1:C:399:LEU:HD12	1:C:439:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:ASP:HB2	1:D:485:THR:HG23	1.97	0.46
1:D:163:THR:HG21	1:D:427:MET:SD	2.56	0.46
1:D:325:ILE:N	1:D:326:PRO:CD	2.78	0.46
1:A:419:LEU:HD22	1:A:421:LYS:HE3	1.96	0.46
1:D:302:ARG:O	1:D:306:ILE:HG13	2.15	0.46
1:B:215:ALA:HA	1:B:220:ASN:O	2.15	0.46
1:A:244:GLU:HA	1:A:270:VAL:O	2.16	0.46
1:B:152:VAL:O	1:B:202:ALA:HB2	2.16	0.46
1:B:301:VAL:HG13	1:B:472:GLU:HB3	1.98	0.46
1:D:322:GLY:O	1:D:326:PRO:HB2	2.15	0.46
1:D:122:PHE:CD1	1:D:122:PHE:C	2.89	0.46
1:B:175:ASN:N	1:B:179:SER:O	2.42	0.46
1:A:368:LYS:HG3	4:A:2006:HOH:O	2.15	0.46
1:D:111:MET:HE2	1:D:122:PHE:HE2	1.81	0.45
1:B:45:ASP:OD2	1:B:47:VAL:HG13	2.16	0.45
1:C:466:VAL:HG12	1:C:467:ASN:N	2.30	0.45
1:B:90:ASN:HD21	1:B:138:GLN:HG3	1.81	0.45
1:B:99:LEU:HD23	1:B:111:MET:CE	2.46	0.45
1:A:259:ILE:HD12	1:B:378:SER:HB3	1.98	0.45
1:C:124:ARG:C	1:C:124:ARG:HD3	2.36	0.45
1:D:511:LYS:H	1:D:511:LYS:HD2	1.82	0.45
1:D:58:THR:HA	1:D:86:THR:O	2.16	0.45
1:D:519:THR:OG1	1:D:520:THR:N	2.49	0.45
1:A:225:LYS:HA	1:A:379:TYR:CD2	2.51	0.45
1:B:301:VAL:HG13	1:B:472:GLU:CB	2.47	0.45
1:D:212:ALA:HB3	1:D:245:VAL:HG12	1.99	0.45
1:A:485:THR:O	1:A:487:ILE:HG23	2.16	0.45
1:C:150:ALA:O	1:D:390:ARG:HD2	2.17	0.45
1:D:326:PRO:HB3	1:D:398:MET:HG2	1.98	0.45
1:B:104:GLN:HE22	1:B:121:GLU:HG2	1.82	0.45
1:D:244:GLU:HA	1:D:270:VAL:O	2.16	0.45
1:A:323:ILE:HG21	1:A:367:GLY:HA3	1.98	0.45
1:A:510:PRO:C	1:A:511:LYS:HD2	2.37	0.45
1:C:472:GLU:HG3	1:C:473:LYS:N	2.32	0.45
1:C:232:LEU:HG	1:C:261:ILE:HD11	1.98	0.45
1:C:191:GLU:HA	1:C:195:GLN:O	2.17	0.45
1:A:235:CYS:O	1:A:241:THR:HG21	2.17	0.45
1:C:486:LEU:HD11	1:C:488:GLU:O	2.17	0.44
1:D:119:ASN:ND2	1:D:119:ASN:C	2.69	0.44
1:C:244:GLU:HA	1:C:270:VAL:O	2.17	0.44
1:C:127:LEU:C	1:C:129:GLY:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:GLU:HG3	1:D:473:LYS:N	2.32	0.44
1:C:152:VAL:O	1:C:202:ALA:HB2	2.17	0.44
1:D:474:ALA:HB1	1:D:486:LEU:CD1	2.48	0.44
1:B:90:ASN:ND2	1:B:138:GLN:HG3	2.32	0.44
1:C:399:LEU:CD1	1:C:439:VAL:HG22	2.47	0.44
1:A:308:ARG:HD3	1:A:516:GLN:O	2.17	0.44
1:B:465:CYS:SG	3:B:9008:EMT:CZ	3.06	0.44
1:B:40:THR:CG2	1:B:219:GLY:HA3	2.35	0.44
1:A:311:LEU:HG	1:A:518:VAL:HG13	1.99	0.44
1:B:228:ARG:HB3	4:B:2065:HOH:O	2.16	0.44
1:A:223:PHE:HE1	1:A:261:ILE:HG12	1.82	0.44
1:B:343:SER:HB2	1:B:350:LEU:HD11	1.99	0.44
1:D:332:PHE:CG	1:D:518:VAL:HG21	2.53	0.44
1:B:489:LEU:O	1:B:515:MET:N	2.51	0.44
1:D:373:VAL:HG22	1:D:377:ALA:CB	2.48	0.44
1:C:180:ILE:N	1:C:180:ILE:CD1	2.80	0.44
3:A:9007:EMT:HE2	4:A:2025:HOH:O	2.55	0.43
1:D:163:THR:CG2	1:D:165:VAL:H	2.13	0.43
1:A:408:GLY:CA	1:A:464:GLN:HA	2.47	0.43
1:D:127:LEU:HD21	1:D:420:VAL:HG21	1.99	0.43
1:C:132:GLU:HA	1:C:172:ILE:O	2.18	0.43
1:D:92:ALA:HB2	1:D:111:MET:HE1	1.99	0.43
1:A:410:LEU:HD23	1:A:462:GLY:O	2.18	0.43
1:B:304:ARG:HG2	1:B:490:TRP:CH2	2.54	0.43
1:C:210:VAL:HG13	1:C:231:ASN:HB3	2.00	0.43
1:D:365:ASN:HB2	4:D:2139:HOH:O	2.19	0.43
1:A:236:LYS:NZ	1:B:384:GLU:OE1	2.50	0.43
1:B:217:GLN:HE21	1:B:217:GLN:HB2	1.66	0.43
1:D:73:LEU:HG	1:D:244:GLU:OE1	2.18	0.43
1:D:511:LYS:CD	1:D:511:LYS:N	2.81	0.43
1:D:442:GLU:HG2	1:D:451:LYS:HZ2	1.84	0.43
1:A:414:MET:HG2	1:A:415:ILE:N	2.34	0.43
1:A:401:ALA:HB3	1:A:439:VAL:HG11	2.01	0.43
1:A:405:SER:HB3	1:A:409:ASP:HB2	2.00	0.43
1:C:301:VAL:HG13	1:C:472:GLU:CB	2.48	0.43
1:B:126:TYR:CE1	1:B:133:VAL:CG1	3.01	0.43
1:D:139:GLY:HA2	1:D:386:PHE:CG	2.54	0.43
1:A:410:LEU:N	1:A:410:LEU:HD23	2.34	0.43
1:A:99:LEU:HD23	1:A:111:MET:HE1	2.00	0.43
1:B:210:VAL:HG13	1:B:231:ASN:HB3	2.00	0.43
1:C:305:ILE:HG22	1:C:325:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:LEU:HG	1:D:261:ILE:HD11	2.00	0.43
1:B:474:ALA:HB1	1:B:486:LEU:HD11	2.00	0.43
1:D:104:GLN:HE21	1:D:104:GLN:N	2.17	0.43
1:A:232:LEU:HB3	1:A:233:PRO:CD	2.49	0.43
1:C:45:ASP:OD2	1:C:47:VAL:CG1	2.67	0.43
1:C:354:PRO:CB	1:C:358:GLU:HB2	2.48	0.42
1:A:482:LYS:O	1:C:271:LYS:HE3	2.20	0.42
1:B:323:ILE:HG21	1:B:367:GLY:HA3	2.01	0.42
1:C:173:LYS:HE2	1:C:182:ILE:HG13	2.01	0.42
1:B:92:ALA:HB2	1:B:111:MET:HE1	2.01	0.42
1:A:480:ARG:HB3	1:A:480:ARG:HH11	1.84	0.42
1:C:225:LYS:HA	1:C:379:TYR:CD2	2.53	0.42
1:A:325:ILE:N	1:A:326:PRO:CD	2.83	0.42
1:D:301:VAL:HG13	1:D:472:GLU:CB	2.48	0.42
1:D:506:PHE:HA	2:D:9000:EMC:C1	2.49	0.42
1:A:506:PHE:HD1	1:A:507:ALA:O	2.02	0.42
1:C:189:VAL:HG22	1:C:198:ILE:HG22	2.02	0.42
1:B:104:GLN:HE21	1:B:104:GLN:CA	2.31	0.42
1:A:45:ASP:OD2	1:A:47:VAL:HG13	2.18	0.42
1:C:130:GLU:OE1	1:C:130:GLU:HA	2.20	0.42
1:D:210:VAL:HG13	1:D:231:ASN:HB3	2.01	0.42
1:B:141:LEU:O	1:B:145:ILE:HG13	2.19	0.42
1:A:509:SER:C	1:A:511:LYS:N	2.73	0.42
1:B:471:THR:HG23	1:B:473:LYS:H	1.84	0.42
1:C:480:ARG:H	1:C:480:ARG:NE	2.17	0.42
1:A:450:HIS:O	1:A:453:MET:HE2	2.19	0.42
1:D:472:GLU:HG3	1:D:473:LYS:H	1.83	0.42
1:C:45:ASP:OD2	1:C:47:VAL:HG13	2.19	0.42
1:B:84:GLU:HA	1:B:109:LYS:HB2	2.02	0.42
1:B:176:LYS:O	1:B:177:ASP:HB3	2.20	0.42
1:C:420:VAL:CB	4:C:2121:HOH:O	2.68	0.42
1:D:166:GLN:HA	1:D:187:ARG:HB2	2.02	0.42
1:B:139:GLY:HA2	1:B:386:PHE:CG	2.55	0.42
1:A:207:PHE:HA	1:A:240:THR:O	2.20	0.42
1:A:215:ALA:CB	1:A:269:LEU:HD21	2.49	0.42
1:A:152:VAL:O	1:A:202:ALA:HB2	2.19	0.42
1:B:45:ASP:OD2	1:B:47:VAL:CG1	2.68	0.42
1:B:472:GLU:HG3	1:B:473:LYS:N	2.35	0.41
1:A:283:SER:O	1:A:354:PRO:HD2	2.20	0.41
1:B:53:ILE:HA	1:B:54:PRO:HD3	1.85	0.41
1:C:489:LEU:CD1	1:C:498:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ALA:HB3	1:C:241:THR:HG22	2.02	0.41
1:A:511:LYS:CD	1:A:511:LYS:N	2.80	0.41
1:C:121:GLU:HA	1:C:121:GLU:OE1	2.19	0.41
1:C:138:GLN:NE2	4:C:2111:HOH:O	2.53	0.41
1:B:77:LEU:HD11	1:B:209:LEU:HD11	2.02	0.41
1:A:210:VAL:HG13	1:A:231:ASN:HB3	2.03	0.41
1:D:446:LYS:HZ2	1:D:449:ALA:HB2	1.85	0.41
1:C:325:ILE:N	1:C:326:PRO:CD	2.84	0.41
1:A:413:TRP:CZ3	1:A:414:MET:HB2	2.55	0.41
1:A:409:ASP:HB3	1:A:460:LEU:CD2	2.50	0.41
1:C:441:MET:HA	4:C:2130:HOH:O	2.20	0.41
1:A:311:LEU:CD2	1:A:518:VAL:HG12	2.50	0.41
1:A:58:THR:HA	1:A:86:THR:O	2.20	0.41
1:C:163:THR:CG2	1:C:165:VAL:HG23	2.51	0.41
1:B:354:PRO:HD3	1:B:371:VAL:HA	2.03	0.41
1:C:367:GLY:O	1:C:368:LYS:CB	2.68	0.41
1:D:412:ASN:ND2	1:D:461:THR:OG1	2.54	0.41
1:D:367:GLY:O	1:D:368:LYS:CB	2.69	0.41
1:B:207:PHE:HA	1:B:240:THR:O	2.21	0.41
1:D:99:LEU:HD23	1:D:111:MET:HE3	2.02	0.41
1:C:127:LEU:C	1:C:129:GLY:N	2.74	0.41
1:C:77:LEU:HD11	1:C:209:LEU:HD11	2.03	0.41
1:D:53:ILE:HA	1:D:54:PRO:HD3	1.86	0.41
1:A:420:VAL:HG23	4:A:2093:HOH:O	2.19	0.41
1:C:223:PHE:HE1	1:C:261:ILE:HG12	1.86	0.41
1:D:47:VAL:HG13	4:D:2003:HOH:O	2.21	0.41
1:D:65:GLY:HA3	1:D:368:LYS:HD2	2.02	0.41
1:D:217:GLN:HB2	1:D:217:GLN:HE21	1.62	0.41
1:A:40:THR:CG2	1:A:219:GLY:HA3	2.39	0.41
1:A:116:VAL:HG21	1:A:122:PHE:CZ	2.56	0.41
1:A:453:MET:HA	1:A:504:CYS:H	1.86	0.40
1:D:403:GLN:NE2	1:D:458:LEU:H	2.19	0.40
1:B:354:PRO:CB	1:B:358:GLU:HB2	2.50	0.40
1:A:217:GLN:HB2	1:A:251:ILE:HG13	2.03	0.40
1:C:256:PRO:HB2	1:D:379:TYR:CE2	2.57	0.40
1:C:509:SER:C	1:C:511:LYS:H	2.24	0.40
1:D:62:GLY:HA3	1:D:231:ASN:OD1	2.21	0.40
1:A:285:ARG:HG2	1:A:353:TYR:O	2.21	0.40
1:C:104:GLN:HE21	1:C:104:GLN:CA	2.35	0.40
1:C:207:PHE:HA	1:C:240:THR:O	2.21	0.40
1:B:324:GLY:O	1:B:328:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PHE:N	1:A:42:PHE:CD1	2.90	0.40
1:C:90:ASN:O	1:C:113:SER:HB3	2.21	0.40
1:C:506:PHE:HD1	1:C:507:ALA:O	2.03	0.40
1:B:225:LYS:HA	1:B:379:TYR:CD2	2.56	0.40
1:B:212:ALA:HB3	1:B:245:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/481 (96%)	438 (94%)	18 (4%)	8 (2%)	11	14
1	B	417/481 (87%)	397 (95%)	16 (4%)	4 (1%)	19	28
1	C	417/481 (87%)	397 (95%)	13 (3%)	7 (2%)	11	14
1	D	460/481 (96%)	438 (95%)	18 (4%)	4 (1%)	21	30
All	All	1758/1924 (91%)	1670 (95%)	65 (4%)	23 (1%)	15	21

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	TRP
1	A	416	PRO
1	A	519	THR
1	B	177	ASP
1	C	177	ASP
1	D	177	ASP
1	D	446	LYS
1	D	519	THR
1	A	419	LEU
1	A	505	ASP

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Mol	Chain	Res	Type
1	B	176	LYS
1	C	119	ASN
1	A	229	ASN
1	A	446	LYS
1	C	176	LYS
1	C	229	ASN
1	D	229	ASN
1	A	412	ASN
1	B	178	GLY
1	B	229	ASN
1	C	170	SER
1	C	178	GLY
1	C	117	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/393 (97%)	363 (95%)	19 (5%)	30	48
1	B	347/393 (88%)	331 (95%)	16 (5%)	33	51
1	C	345/393 (88%)	327 (95%)	18 (5%)	29	45
1	D	378/393 (96%)	354 (94%)	24 (6%)	22	35
All	All	1452/1572 (92%)	1375 (95%)	77 (5%)	28	44

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	58	THR
1	A	103	LEU
1	A	104	GLN
1	A	119	ASN
1	A	136	THR
1	A	282	LEU
1	A	325	ILE

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Mol	Chain	Res	Type
1	A	368	LYS
1	A	373	VAL
1	A	399	LEU
1	A	416	PRO
1	A	420	VAL
1	A	446	LYS
1	A	455	LYS
1	A	480	ARG
1	A	485	THR
1	A	504	CYS
1	A	519	THR
1	B	40	THR
1	B	58	THR
1	B	103	LEU
1	B	104	GLN
1	B	119	ASN
1	B	124	ARG
1	B	136	THR
1	B	175	ASN
1	B	176	LYS
1	B	221	VAL
1	B	325	ILE
1	B	368	LYS
1	B	373	VAL
1	B	399	LEU
1	B	480	ARG
1	B	485	THR
1	C	40	THR
1	C	58	THR
1	C	103	LEU
1	C	104	GLN
1	C	136	THR
1	C	166	GLN
1	C	176	LYS
1	C	221	VAL
1	C	235	CYS
1	C	325	ILE
1	C	368	LYS
1	C	373	VAL
1	C	399	LEU
1	C	420	VAL
1	C	480	ARG

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Mol	Chain	Res	Type
1	C	485	THR
1	C	517	GLN
1	C	518	VAL
1	D	40	THR
1	D	58	THR
1	D	103	LEU
1	D	104	GLN
1	D	119	ASN
1	D	133	VAL
1	D	136	THR
1	D	163	THR
1	D	235	CYS
1	D	282	LEU
1	D	325	ILE
1	D	368	LYS
1	D	373	VAL
1	D	399	LEU
1	D	412	ASN
1	D	419	LEU
1	D	423	MET
1	D	446	LYS
1	D	455	LYS
1	D	457	THR
1	D	465	CYS
1	D	480	ARG
1	D	485	THR
1	D	518	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	90	ASN
1	A	104	GLN
1	A	119	ASN
1	A	125	GLN
1	A	166	GLN
1	A	175	ASN
1	A	217	GLN
1	A	393	HIS
1	A	403	GLN
1	B	72	ASN

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Mol	Chain	Res	Type
1	B	90	ASN
1	B	104	GLN
1	B	119	ASN
1	B	125	GLN
1	B	175	ASN
1	B	217	GLN
1	B	393	HIS
1	C	72	ASN
1	C	90	ASN
1	C	104	GLN
1	C	125	GLN
1	C	138	GLN
1	C	166	GLN
1	C	217	GLN
1	C	393	HIS
1	C	516	GLN
1	D	72	ASN
1	D	90	ASN
1	D	104	GLN
1	D	119	ASN
1	D	125	GLN
1	D	138	GLN
1	D	175	ASN
1	D	217	GLN
1	D	393	HIS
1	D	403	GLN
1	D	412	ASN
1	D	464	GLN
1	D	516	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EMC	A	9003	1	1,2,2	0.43	0	0,1,1	0.00	-
3	EMT	A	9007	-	9,13,13	0.92	1 (11%)	8,16,16	0.53	0
2	EMC	B	9004	1	1,2,2	0.54	0	0,1,1	0.00	-
3	EMT	B	9008	-	9,13,13	0.76	0	8,16,16	0.52	0
2	EMC	C	9005	1,4	1,2,2	1.59	0	0,1,1	0.00	-
2	EMC	C	9006	1	1,2,2	0.57	0	0,1,1	0.00	-
2	EMC	D	9000	1	1,2,2	0.60	0	0,1,1	0.00	-
2	EMC	D	9001	1	1,2,2	3.69	1 (100%)	0,1,1	0.00	-
2	EMC	D	9002	1	1,2,2	0.47	0	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EMC	A	9003	1	-	0/0/0/0	0/0/0/0
3	EMT	A	9007	-	-	0/0/8/8	0/1/1/1
2	EMC	B	9004	1	-	0/0/0/0	0/0/0/0
3	EMT	B	9008	-	-	0/0/8/8	0/1/1/1
2	EMC	C	9005	1,4	-	0/0/0/0	0/0/0/0
2	EMC	C	9006	1	-	0/0/0/0	0/0/0/0
2	EMC	D	9000	1	-	0/0/0/0	0/0/0/0
2	EMC	D	9001	1	-	0/0/0/0	0/0/0/0
2	EMC	D	9002	1	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9001	EMC	C2-C1	-3.69	1.30	1.49
3	A	9007	EMT	CE1-SD	2.14	1.82	1.78

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9007	EMT	9	0
3	B	9008	EMT	8	0
2	D	9000	EMC	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	468/481 (97%)	1.23	98 (20%)	1	1	23, 41, 73, 83	0
1	B	425/481 (88%)	1.19	84 (19%)	1	1	24, 44, 76, 82	0
1	C	425/481 (88%)	1.12	77 (18%)	2	2	19, 40, 77, 86	0
1	D	464/481 (96%)	1.09	81 (17%)	2	2	18, 36, 62, 80	0
All	All	1782/1924 (92%)	1.16	340 (19%)	2	1	18, 40, 75, 86	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	520	THR	14.0
1	A	510	PRO	8.4
1	B	481	LYS	8.2
1	A	419	LEU	8.0
1	C	480	ARG	8.0
1	D	352	PRO	7.5
1	A	457	THR	7.5
1	A	417	GLY	7.3
1	B	480	ARG	7.1
1	D	356	GLN	6.9
1	C	503	GLY	6.5
1	B	300	ASN	6.4
1	C	177	ASP	6.3
1	B	178	GLY	6.2
1	A	445	ALA	6.2
1	C	179	SER	6.1
1	D	334	SER	6.1
1	C	481	LYS	6.0
1	A	458	LEU	6.0
1	A	446	LYS	6.0
1	A	336	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	416	PRO	5.9
1	A	449	ALA	5.8
1	D	282	LEU	5.7
1	A	286	LYS	5.7
1	A	511	LYS	5.6
1	C	494	THR	5.5
1	A	335	PRO	5.5
1	B	336	ASN	5.4
1	A	519	THR	5.4
1	D	281	ARG	5.4
1	C	479	ASP	5.4
1	C	336	ASN	5.3
1	B	335	PRO	5.3
1	A	455	LYS	5.3
1	A	450	HIS	5.3
1	B	482	LYS	5.1
1	B	500	LYS	5.1
1	D	332	PHE	5.1
1	D	520	THR	5.0
1	C	504	CYS	5.0
1	D	353	TYR	5.0
1	C	127	LEU	4.9
1	A	454	GLU	4.9
1	A	512	LEU	4.8
1	B	478	VAL	4.8
1	A	334	SER	4.7
1	C	502	THR	4.7
1	D	446	LYS	4.7
1	D	279	ILE	4.7
1	B	491	GLU	4.7
1	A	480	ARG	4.7
1	A	420	VAL	4.7
1	D	355	LEU	4.7
1	D	327	LEU	4.6
1	B	177	ASP	4.6
1	B	520	THR	4.6
1	C	126	TYR	4.6
1	B	511	LYS	4.5
1	D	357	ASN	4.5
1	C	505	ASP	4.5
1	A	514	PRO	4.5
1	A	496	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	510	PRO	4.5
1	D	277	LYS	4.4
1	B	497	ASP	4.4
1	A	447	GLY	4.4
1	A	301	VAL	4.3
1	A	448	ASN	4.3
1	D	300	ASN	4.3
1	C	492	GLY	4.3
1	C	499	LYS	4.3
1	B	301	VAL	4.3
1	B	487	ILE	4.3
1	A	337	MET	4.3
1	A	470	ILE	4.2
1	A	415	ILE	4.2
1	A	459	PRO	4.2
1	C	301	VAL	4.2
1	A	315	ASP	4.2
1	D	482	LYS	4.1
1	D	445	ALA	4.1
1	B	479	ASP	4.1
1	B	490	TRP	4.1
1	D	329	ALA	4.1
1	A	283	SER	4.0
1	D	325	ILE	4.0
1	A	333	ILE	4.0
1	C	498	ILE	4.0
1	D	480	ARG	3.9
1	A	490	TRP	3.9
1	C	483	GLY	3.9
1	C	500	LYS	3.8
1	C	482	LYS	3.8
1	C	493	LEU	3.8
1	B	420	VAL	3.8
1	C	490	TRP	3.8
1	C	178	GLY	3.8
1	C	175	ASN	3.8
1	D	316	GLY	3.7
1	D	178	GLY	3.7
1	C	300	ASN	3.7
1	A	250	ASP	3.7
1	D	324	GLY	3.7
1	D	336	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	335	PRO	3.7
1	C	510	PRO	3.7
1	B	519	THR	3.7
1	D	328	LEU	3.7
1	B	433	ALA	3.6
1	D	303	GLU	3.6
1	A	504	CYS	3.6
1	A	466	VAL	3.6
1	D	359	VAL	3.6
1	A	99	LEU	3.6
1	C	124	ARG	3.6
1	A	491	GLU	3.6
1	A	421	LYS	3.6
1	A	492	GLY	3.5
1	B	505	ASP	3.5
1	C	484	LEU	3.5
1	A	475	VAL	3.5
1	A	277	LYS	3.5
1	A	481	LYS	3.5
1	B	302	ARG	3.5
1	C	123	GLU	3.5
1	C	501	SER	3.5
1	A	357	ASN	3.5
1	A	284	VAL	3.5
1	B	180	ILE	3.5
1	B	315	ASP	3.5
1	D	326	PRO	3.4
1	A	328	LEU	3.4
1	B	483	GLY	3.4
1	C	465	CYS	3.4
1	C	506	PHE	3.4
1	C	117	GLY	3.4
1	D	449	ALA	3.4
1	C	473	LYS	3.4
1	C	478	VAL	3.4
1	D	354	PRO	3.4
1	C	122	PHE	3.4
1	B	518	VAL	3.3
1	C	514	PRO	3.3
1	A	456	CYS	3.3
1	D	315	ASP	3.3
1	D	448	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	497	ASP	3.2
1	A	485	THR	3.2
1	B	337	MET	3.2
1	B	328	LEU	3.2
1	D	410	LEU	3.2
1	A	508	VAL	3.2
1	B	421	LYS	3.2
1	C	511	LYS	3.2
1	A	493	LEU	3.2
1	D	447	GLY	3.2
1	D	177	ASP	3.1
1	A	513	ILE	3.1
1	C	217	GLN	3.1
1	C	176	LYS	3.1
1	A	282	LEU	3.1
1	A	413	TRP	3.1
1	C	181	ALA	3.1
1	B	494	THR	3.1
1	C	420	VAL	3.0
1	A	465	CYS	3.0
1	D	323	ILE	3.0
1	A	356	GLN	3.0
1	B	503	GLY	2.9
1	C	495	VAL	2.9
1	C	441	MET	2.9
1	B	169	GLY	2.9
1	D	117	GLY	2.9
1	D	476	PHE	2.9
1	D	483	GLY	2.9
1	B	142	ALA	2.9
1	D	469	ILE	2.9
1	B	484	LEU	2.9
1	C	334	SER	2.9
1	D	475	VAL	2.9
1	B	96	ASN	2.9
1	A	409	ASP	2.9
1	C	518	VAL	2.9
1	A	332	PHE	2.9
1	B	104	GLN	2.9
1	C	485	THR	2.9
1	B	176	LYS	2.8
1	B	496	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	496	ASP	2.8
1	B	181	ALA	2.8
1	B	485	THR	2.8
1	A	355	LEU	2.8
1	A	399	LEU	2.8
1	D	322	GLY	2.8
1	A	353	TYR	2.8
1	B	195	GLN	2.8
1	D	365	ASN	2.8
1	B	277	LYS	2.8
1	A	516	GLN	2.8
1	C	84	GLU	2.8
1	D	335	PRO	2.8
1	B	286	LYS	2.8
1	D	479	ASP	2.8
1	B	465	CYS	2.7
1	C	125	GLN	2.7
1	C	130	GLU	2.7
1	A	453	MET	2.7
1	D	115	TYR	2.7
1	C	472	GLU	2.7
1	B	179	SER	2.7
1	C	307	LYS	2.7
1	A	503	GLY	2.7
1	C	193	ASN	2.7
1	B	333	ILE	2.7
1	D	470	ILE	2.7
1	A	460	LEU	2.7
1	D	337	MET	2.7
1	A	444	SER	2.6
1	D	471	THR	2.6
1	A	476	PHE	2.6
1	B	508	VAL	2.6
1	C	491	GLU	2.6
1	D	481	LYS	2.6
1	D	301	VAL	2.6
1	D	333	ILE	2.6
1	B	514	PRO	2.6
1	D	116	VAL	2.6
1	B	184	SER	2.6
1	C	282	LEU	2.6
1	C	512	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	439	VAL	2.6
1	B	283	SER	2.5
1	D	194	GLY	2.5
1	A	506	PHE	2.5
1	A	405	SER	2.5
1	A	302	ARG	2.5
1	C	128	ALA	2.5
1	B	375	PRO	2.5
1	B	355	LEU	2.5
1	B	498	ILE	2.5
1	C	170	SER	2.5
1	D	330	SER	2.5
1	C	475	VAL	2.5
1	B	161	TYR	2.5
1	A	324	GLY	2.5
1	D	193	ASN	2.5
1	A	402	MET	2.5
1	A	253	SER	2.5
1	D	358	GLU	2.5
1	A	249	VAL	2.5
1	A	321	LEU	2.5
1	B	470	ILE	2.5
1	C	173	LYS	2.4
1	D	511	LYS	2.4
1	A	438	VAL	2.4
1	C	182	ILE	2.4
1	B	165	VAL	2.4
1	B	47	VAL	2.4
1	C	332	PHE	2.4
1	B	129	GLY	2.4
1	A	285	ARG	2.4
1	B	250	ASP	2.4
1	C	329	ALA	2.4
1	B	506	PHE	2.4
1	A	501	SER	2.4
1	D	456	CYS	2.4
1	A	161	TYR	2.4
1	A	462	GLY	2.4
1	C	174	TYR	2.4
1	B	434	LYS	2.3
1	B	162	GLY	2.3
1	D	369	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	508	VAL	2.3
1	B	44	THR	2.3
1	C	51	LYS	2.3
1	B	233	PRO	2.3
1	B	400	GLY	2.3
1	B	502	THR	2.3
1	D	196	HIS	2.3
1	A	418	LYS	2.3
1	D	421	LYS	2.3
1	C	116	VAL	2.3
1	A	352	PRO	2.3
1	B	381	SER	2.3
1	D	370	THR	2.3
1	D	351	GLY	2.3
1	D	404	VAL	2.3
1	B	509	SER	2.3
1	A	437	VAL	2.3
1	B	276	GLU	2.2
1	D	491	GLU	2.2
1	B	193	ASN	2.2
1	D	420	VAL	2.2
1	A	326	PRO	2.2
1	A	518	VAL	2.2
1	D	111	MET	2.2
1	B	61	VAL	2.2
1	A	111	MET	2.2
1	C	513	ILE	2.2
1	A	351	GLY	2.2
1	B	182	ILE	2.2
1	D	500	LYS	2.2
1	D	61	VAL	2.2
1	A	498	ILE	2.2
1	B	84	GLU	2.2
1	D	314	GLU	2.2
1	C	309	ALA	2.1
1	C	520	THR	2.1
1	D	191	GLU	2.1
1	A	400	GLY	2.1
1	D	437	VAL	2.1
1	B	127	LEU	2.1
1	D	438	VAL	2.1
1	A	497	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	235	CYS	2.1
1	D	360	ASP	2.1
1	C	196	HIS	2.1
1	D	505	ASP	2.1
1	B	331	ASN	2.1
1	D	430	VAL	2.1
1	D	478	VAL	2.1
1	B	124	ARG	2.1
1	B	499	LYS	2.1
1	A	83	LYS	2.0
1	D	364	ILE	2.0
1	A	505	ASP	2.0
1	B	163	THR	2.0
1	B	471	THR	2.0
1	D	338	THR	2.0
1	C	56	GLY	2.0
1	D	180	ILE	2.0
1	B	486	LEU	2.0
1	B	504	CYS	2.0
1	A	61	VAL	2.0
1	B	194	GLY	2.0
1	C	351	GLY	2.0
1	A	89	SER	2.0
1	A	489	LEU	2.0
1	A	397	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	EMC	D	9001	3/3	-0.05	0.71	13.91	2,2,2,11	3
2	EMC	D	9002	3/3	0.78	0.70	11.17	25,25,25,27	3
2	EMC	A	9003	3/3	0.81	0.66	9.49	23,23,23,25	3
3	EMT	B	9008	13/13	0.28	0.60	6.49	32,41,45,47	13
3	EMT	A	9007	13/13	0.58	0.63	5.65	5,11,12,13	13
2	EMC	D	9000	3/3	0.66	0.59	2.97	46,46,47,48	3
2	EMC	B	9004	3/3	0.82	0.60	-	42,42,44,45	3
2	EMC	C	9006	3/3	0.52	0.51	-	65,65,65,69	3
2	EMC	C	9005	3/3	0.64	0.58	-	2,2,2,5	3

6.5 Other polymers

There are no such residues in this entry.